



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 5, 2016 – 11:22 AM EDT

PDB ID : 5JSA  
Title : Uncleaved prefusion optimized gp140 trimer with an engineered 10-residue HR1 turn bound to broadly neutralizing antibodies 8ANC195 and PGT128  
Authors : Kong, L.; Wilson, I.A.  
Deposited on : 2016-05-07  
Resolution : 6.31 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027790

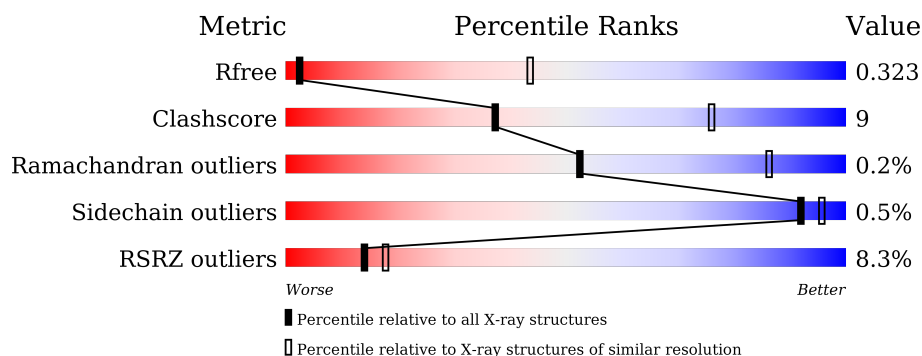
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1008 (8.90-3.66)
Clashscore	102246	1056 (8.90-3.70)
Ramachandran outliers	100387	1029 (8.90-3.66)
Sidechain outliers	100360	1001 (8.90-3.66)
RSRZ outliers	91569	1007 (8.90-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	239	<div> <div>17%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div></div> </div> </div>
2	B	211	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div></div> </div> </div>
3	C	480	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>7%</div> </div> </div>
4	D	142	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>7%</div> </div> </div>
5	E	238	<div> <div>14%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>6%</div> </div> </div>
6	F	215	<div> <div>8%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div></div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	C	603	-	-	-	X
7	NAG	C	616	-	-	-	X
7	NAG	E	301	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12075 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called broadly neutralizing antibody PGT128 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1735	1105	292	332	6			

- Molecule 2 is a protein called broadly neutralizing antibody PGT128 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1514	950	254	306	4			

- Molecule 3 is a protein called gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3519	2210	622	659	28			

- Molecule 4 is a protein called gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	132	Total	C	N	O	S	0	0	0
			1052	663	178	205	6			

- Molecule 5 is a protein called broadly neutralizing antibody 8ANC195 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	224	Total	C	N	O	S	0	0	0
			1686	1072	284	325	5			

- Molecule 6 is a protein called broadly neutralizing antibody 8ANC195 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	212	Total	C	N	O	S	0	0	0
			1626	1018	279	324	5			

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

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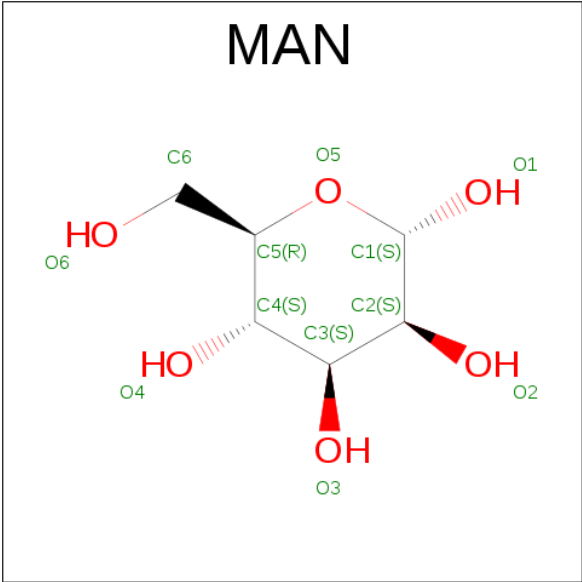
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		
8	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		

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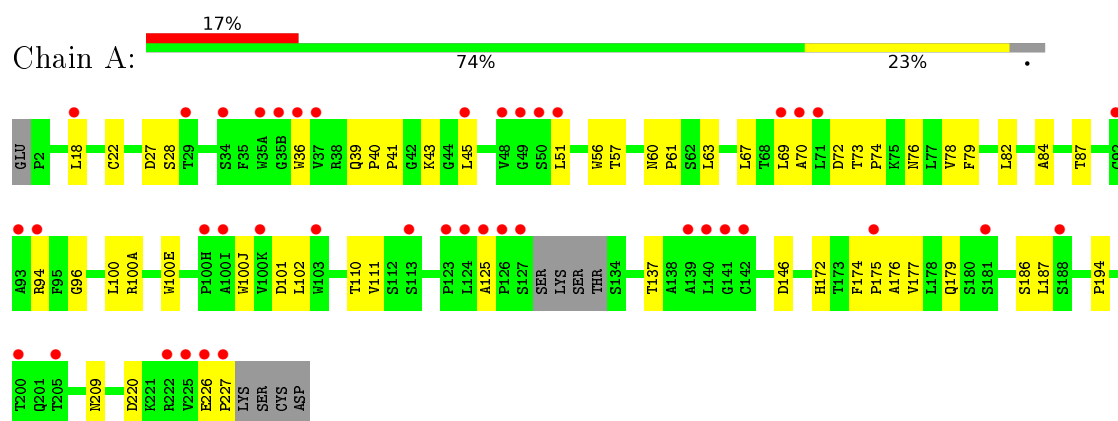
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	D	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		

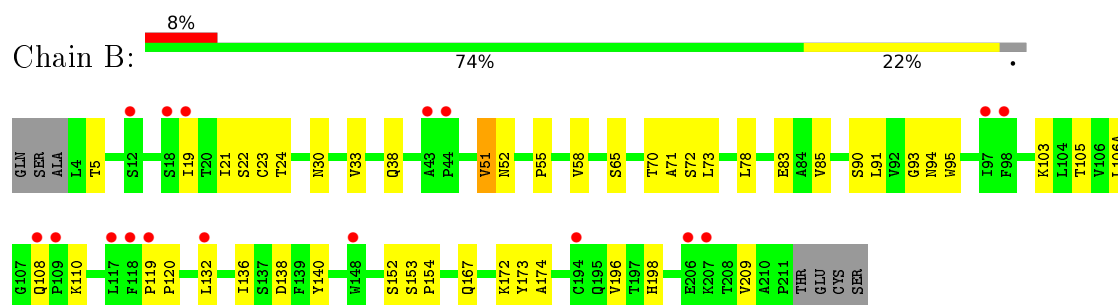
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

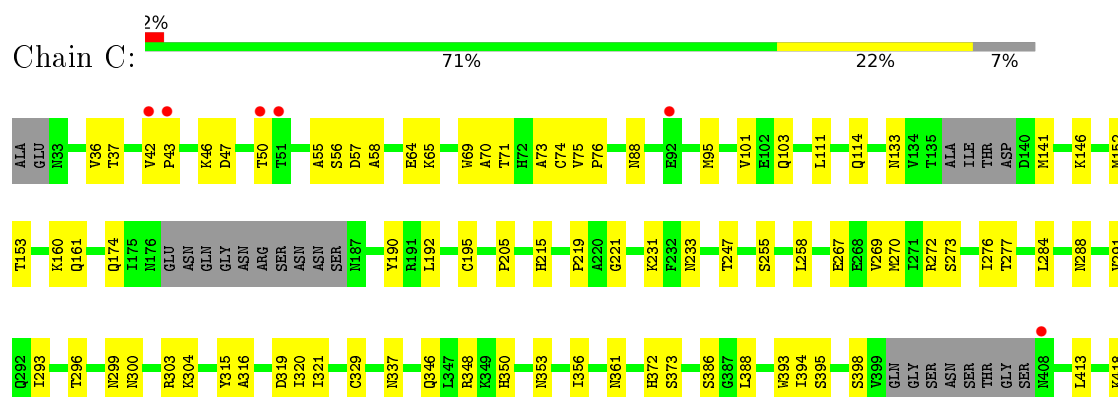
- Molecule 1: broadly neutralizing antibody PGT128 heavy chain

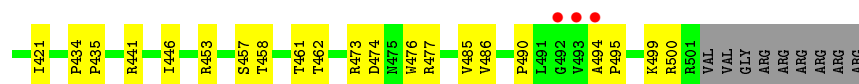


- Molecule 2: broadly neutralizing antibody PGT128 light chain



- Molecule 3: gp120

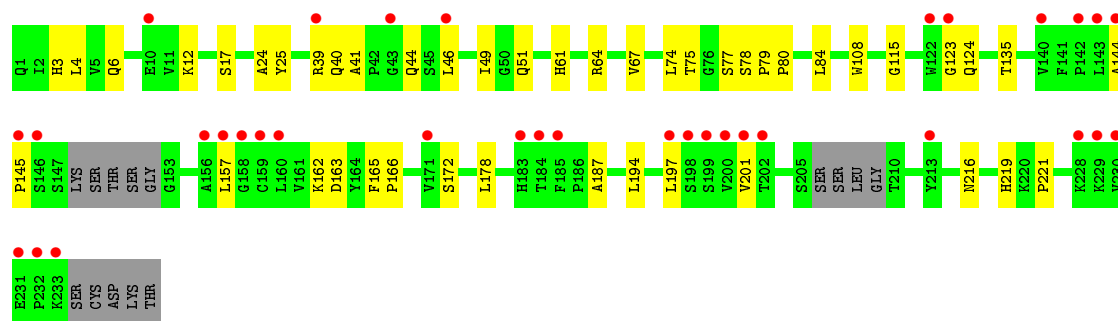
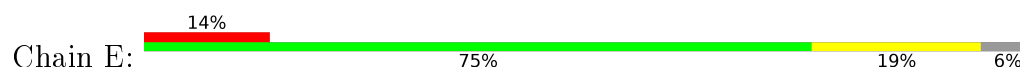




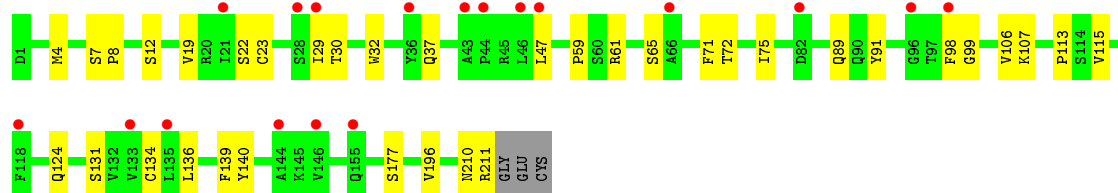
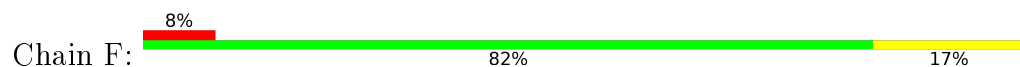
- Molecule 4: gp41



- Molecule 5: broadly neutralizing antibody 8ANC195 heavy chain



- Molecule 6: broadly neutralizing antibody 8ANC195 light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	266.28Å 266.28Å 266.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.14 – 6.31 47.07 – 6.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.14-6.31) 99.9 (47.07-6.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 6.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.281 , 0.322 0.281 , 0.323	Depositor DCC
$R_{free}$ test set	682 reflections (9.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	357.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 305.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.049 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	12075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	350.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.20	0/1786	0.40	0/2449
2	B	0.21	0/1552	0.44	1/2121 (0.0%)
3	C	0.22	0/3592	0.42	0/4875
4	D	0.27	0/1072	0.58	1/1458 (0.1%)
5	E	0.21	0/1730	0.39	0/2361
6	F	0.22	0/1661	0.40	0/2256
All	All	0.22	0/11393	0.43	2/15520 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	545	LEU	CA-CB-CG	8.87	135.71	115.30
2	B	108	GLN	C-N-CD	-6.56	106.17	120.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1735	0	1690	37	0
2	B	1514	0	1473	35	0
3	C	3519	0	3461	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1052	0	1017	37	1
5	E	1686	0	1658	30	0
6	F	1626	0	1581	27	0
7	C	378	0	328	8	0
7	D	42	0	37	2	0
7	E	28	0	24	0	0
8	C	110	0	91	0	0
8	D	11	0	9	1	0
8	E	11	0	8	0	0
9	C	264	0	225	7	0
9	D	11	0	10	0	0
9	E	88	0	72	0	0
All	All	12075	0	11684	220	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 220 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:TRP:HE1	9:C:625:MAN:HO4	1.12	0.93
4:D:553:ASP:OD1	4:D:564:GLN:NE2	2.07	0.85
3:C:499:LYS:HG2	3:C:500:ARG:H	1.50	0.77
2:B:95:TRP:NE1	9:C:625:MAN:O4	2.16	0.75
3:C:394:ILE:HG22	3:C:395:SER:H	1.53	0.72

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:546:SER:OG	4:D:580:GLN:OE1[5_555]	2.09	0.11

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/239 (95%)	212 (94%)	14 (6%)	0	100	100
2	B	202/211 (96%)	194 (96%)	7 (4%)	1 (0%)	34	76
3	C	439/480 (92%)	417 (95%)	22 (5%)	0	100	100
4	D	130/142 (92%)	119 (92%)	9 (7%)	2 (2%)	13	57
5	E	218/238 (92%)	209 (96%)	9 (4%)	0	100	100
6	F	210/215 (98%)	205 (98%)	5 (2%)	0	100	100
All	All	1425/1525 (93%)	1356 (95%)	66 (5%)	3 (0%)	52	86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	552	ILE
2	B	51	VAL
4	D	555	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/203 (96%)	194 (100%)	0	100	100
2	B	171/177 (97%)	170 (99%)	1 (1%)	90	95
3	C	399/426 (94%)	396 (99%)	3 (1%)	86	94
4	D	115/120 (96%)	113 (98%)	2 (2%)	68	87
5	E	192/204 (94%)	192 (100%)	0	100	100
6	F	180/182 (99%)	180 (100%)	0	100	100
All	All	1251/1312 (95%)	1245 (100%)	6 (0%)	92	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	303	ARG
4	D	563	LYS
3	C	337	ASN
3	C	233	ASN
4	D	562	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	114	GLN
3	C	194	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

77 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	C	601	3,7	14,14,15	0.28	0	15,19,21	0.55	0
7	NAG	C	602	7	14,14,15	0.18	0	15,19,21	0.28	0
7	NAG	C	603	3,7	14,14,15	0.21	0	15,19,21	0.34	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	C	604	7	14,14,15	0.27	0	15,19,21	0.32	0
7	NAG	C	605	3,7	14,14,15	0.21	0	15,19,21	1.03	1 (6%)
7	NAG	C	606	7	14,14,15	0.22	0	15,19,21	0.27	0
7	NAG	C	607	3,7	14,14,15	0.59	0	15,19,21	0.42	0
7	NAG	C	608	8,7	14,14,15	0.57	0	15,19,21	0.43	0
8	BMA	C	609	9,7	11,11,12	0.53	0	15,15,17	0.70	0
9	MAN	C	610	9,8	11,11,12	0.69	0	15,15,17	1.06	1 (6%)
9	MAN	C	611	9	11,11,12	0.57	0	15,15,17	1.00	1 (6%)
9	MAN	C	612	9,8	11,11,12	0.87	0	15,15,17	0.90	1 (6%)
9	MAN	C	613	9	11,11,12	0.76	1 (9%)	15,15,17	1.40	2 (13%)
9	MAN	C	614	9	11,11,12	0.61	0	15,15,17	1.00	2 (13%)
7	NAG	C	615	3	14,14,15	0.34	0	15,19,21	0.26	0
7	NAG	C	616	3,7	14,14,15	0.24	0	15,19,21	0.38	0
7	NAG	C	617	8,7	14,14,15	0.22	0	15,19,21	0.29	0
9	MAN	C	618	9	11,11,12	0.65	0	15,15,17	1.21	2 (13%)
9	MAN	C	619	9	11,11,12	0.67	0	15,15,17	0.90	1 (6%)
8	BMA	C	620	9,7	11,11,12	0.79	0	15,15,17	0.88	0
9	MAN	C	621	9,8	11,11,12	0.71	1 (9%)	15,15,17	1.11	2 (13%)
9	MAN	C	622	9,8	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
9	MAN	C	623	9	11,11,12	0.65	0	15,15,17	0.98	2 (13%)
9	MAN	C	624	9	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
9	MAN	C	625	9	11,11,12	0.78	0	15,15,17	0.96	1 (6%)
7	NAG	C	626	3,7	14,14,15	0.50	0	15,19,21	0.55	0
7	NAG	C	627	8,7	14,14,15	0.19	0	15,19,21	0.66	0
8	BMA	C	628	9,7	11,11,12	0.80	0	15,15,17	1.07	1 (6%)
9	MAN	C	629	9,8	11,11,12	0.69	0	15,15,17	0.95	2 (13%)
9	MAN	C	630	9	11,11,12	0.65	0	15,15,17	0.96	1 (6%)
9	MAN	C	631	9	11,11,12	0.60	0	15,15,17	0.99	2 (13%)
9	MAN	C	632	9,8	11,11,12	0.73	0	15,15,17	1.29	2 (13%)
9	MAN	C	633	9	11,11,12	0.57	0	15,15,17	1.10	2 (13%)
9	MAN	C	634	9	11,11,12	0.57	0	15,15,17	1.11	2 (13%)
7	NAG	C	635	3,7	14,14,15	0.29	0	15,19,21	0.41	0
7	NAG	C	636	8,7	14,14,15	0.40	0	15,19,21	0.44	0
8	BMA	C	637	9,7	11,11,12	0.64	0	15,15,17	1.00	1 (6%)
9	MAN	C	638	8	11,11,12	0.73	1 (9%)	15,15,17	1.15	2 (13%)
9	MAN	C	639	9,8	11,11,12	0.66	0	15,15,17	1.27	1 (6%)
9	MAN	C	640	9	11,11,12	0.51	0	15,15,17	1.10	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	C	641	9	11,11,12	0.63	0	15,15,17	1.22	2 (13%)
7	NAG	C	642	3,7	14,14,15	0.46	0	15,19,21	0.37	0
7	NAG	C	643	8,7	14,14,15	0.23	0	15,19,21	0.55	0
8	BMA	C	644	9,7	11,11,12	0.64	0	15,15,17	1.25	1 (6%)
9	MAN	C	645	9,8	11,11,12	0.59	0	15,15,17	1.30	2 (13%)
9	MAN	C	646	9	11,11,12	0.22	0	15,15,17	0.52	0
7	NAG	C	647	3,7	14,14,15	0.40	0	15,19,21	0.29	0
7	NAG	C	648	8,7	14,14,15	0.26	0	15,19,21	0.59	0
8	BMA	C	649	7	11,11,12	0.63	0	15,15,17	0.77	0
7	NAG	C	650	3,7	14,14,15	0.30	0	15,19,21	0.43	0
7	NAG	C	651	8,7	14,14,15	0.37	0	15,19,21	0.59	0
8	BMA	C	652	7	11,11,12	0.65	0	15,15,17	0.78	0
7	NAG	C	653	3,7	14,14,15	0.29	0	15,19,21	0.66	0
7	NAG	C	654	8,7	14,14,15	0.23	0	15,19,21	0.63	0
8	BMA	C	655	7	11,11,12	0.62	0	15,15,17	0.75	0
7	NAG	C	656	3,7	14,14,15	0.31	0	15,19,21	0.44	0
7	NAG	C	657	8,7	14,14,15	0.38	0	15,19,21	0.59	0
8	BMA	C	658	7	11,11,12	0.66	0	15,15,17	0.78	0
7	NAG	C	659	3,7	14,14,15	0.31	0	15,19,21	0.44	0
7	NAG	C	660	8,7	14,14,15	0.38	0	15,19,21	0.58	0
8	BMA	C	661	7	11,11,12	0.65	0	15,15,17	0.78	0
7	NAG	D	701	4,7	14,14,15	0.25	0	15,19,21	0.32	0
7	NAG	D	702	8,7	14,14,15	0.40	0	15,19,21	1.43	2 (13%)
8	BMA	D	703	9,7	11,11,12	0.73	0	15,15,17	1.00	0
9	MAN	D	704	8	11,11,12	1.54	3 (27%)	15,15,17	1.33	2 (13%)
7	NAG	D	705	4	14,14,15	0.19	0	15,19,21	0.32	0
7	NAG	E	301	3,7	14,14,15	0.17	0	15,19,21	0.28	0
7	NAG	E	302	8,7	14,14,15	0.37	0	15,19,21	0.38	0
8	BMA	E	303	9,7	11,11,12	0.51	0	15,15,17	0.70	0
9	MAN	E	304	9,8	11,11,12	0.50	0	15,15,17	1.08	2 (13%)
9	MAN	E	305	9	11,11,12	0.72	0	15,15,17	1.07	0
9	MAN	E	306	9	11,11,12	0.53	0	15,15,17	0.97	2 (13%)
9	MAN	E	307	9,8	11,11,12	0.56	0	15,15,17	1.13	2 (13%)
9	MAN	E	308	9	11,11,12	0.60	0	15,15,17	1.16	2 (13%)
9	MAN	E	309	9	11,11,12	0.84	0	15,15,17	1.41	3 (20%)
9	MAN	E	310	9,5	11,11,12	0.65	0	15,15,17	0.94	2 (13%)
9	MAN	E	311	9	11,11,12	0.56	0	15,15,17	1.01	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	601	3,7	-	1/6/23/26	0/1/1/1
7	NAG	C	602	7	-	0/6/23/26	0/1/1/1
7	NAG	C	603	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	604	7	-	0/6/23/26	0/1/1/1
7	NAG	C	605	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	606	7	-	0/6/23/26	0/1/1/1
7	NAG	C	607	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	608	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	609	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	610	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	611	9	-	0/2/19/22	0/1/1/1
9	MAN	C	612	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	613	9	-	0/2/19/22	0/1/1/1
9	MAN	C	614	9	-	0/2/19/22	0/1/1/1
7	NAG	C	615	3	-	0/6/23/26	0/1/1/1
7	NAG	C	616	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	617	8,7	-	0/6/23/26	0/1/1/1
9	MAN	C	618	9	-	0/2/19/22	0/1/1/1
9	MAN	C	619	9	-	0/2/19/22	0/1/1/1
8	BMA	C	620	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	621	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	622	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	623	9	-	0/2/19/22	0/1/1/1
9	MAN	C	624	9	-	0/2/19/22	0/1/1/1
9	MAN	C	625	9	-	0/2/19/22	0/1/1/1
7	NAG	C	626	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	627	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	628	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	629	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	630	9	-	0/2/19/22	0/1/1/1
9	MAN	C	631	9	-	0/2/19/22	0/1/1/1
9	MAN	C	632	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	633	9	-	0/2/19/22	0/1/1/1
9	MAN	C	634	9	-	0/2/19/22	0/1/1/1
7	NAG	C	635	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	636	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	637	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	638	8	-	0/2/19/22	0/1/1/1
9	MAN	C	639	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	640	9	-	0/2/19/22	0/1/1/1
9	MAN	C	641	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	642	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	643	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	644	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	645	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	646	9	-	0/2/19/22	0/1/1/1
7	NAG	C	647	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	648	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	649	7	-	0/2/19/22	0/1/1/1
7	NAG	C	650	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	651	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	652	7	-	0/2/19/22	0/1/1/1
7	NAG	C	653	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	654	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	655	7	-	0/2/19/22	0/1/1/1
7	NAG	C	656	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	657	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	658	7	-	0/2/19/22	0/1/1/1
7	NAG	C	659	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	660	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	661	7	-	0/2/19/22	0/1/1/1
7	NAG	D	701	4,7	-	0/6/23/26	0/1/1/1
7	NAG	D	702	8,7	-	0/6/23/26	0/1/1/1
8	BMA	D	703	9,7	-	0/2/19/22	0/1/1/1
9	MAN	D	704	8	-	0/2/19/22	0/1/1/1
7	NAG	D	705	4	-	0/6/23/26	0/1/1/1
7	NAG	E	301	3,7	-	0/6/23/26	0/1/1/1
7	NAG	E	302	8,7	-	0/6/23/26	0/1/1/1
8	BMA	E	303	9,7	-	0/2/19/22	0/1/1/1
9	MAN	E	304	9,8	-	0/2/19/22	0/1/1/1
9	MAN	E	305	9	-	0/2/19/22	0/1/1/1
9	MAN	E	306	9	-	0/2/19/22	0/1/1/1
9	MAN	E	307	9,8	-	0/2/19/22	0/1/1/1
9	MAN	E	308	9	-	0/2/19/22	0/1/1/1
9	MAN	E	309	9	-	0/2/19/22	0/1/1/1
9	MAN	E	310	9,5	-	0/2/19/22	0/1/1/1
9	MAN	E	311	9	-	0/2/19/22	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	621	MAN	C1-C2	2.01	1.57	1.52
9	C	613	MAN	C1-C2	2.08	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	638	MAN	C1-C2	2.14	1.57	1.52
9	D	704	MAN	C1-C2	2.48	1.58	1.52
9	D	704	MAN	O2-C2	2.60	1.49	1.43

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	309	MAN	O2-C2-C3	-3.29	103.55	110.19
9	C	624	MAN	O2-C2-C3	-3.14	103.86	110.19
9	C	618	MAN	O2-C2-C3	-2.98	104.18	110.19
8	C	637	BMA	C1-C2-C3	-2.80	106.16	109.55
9	E	311	MAN	O2-C2-C3	-2.49	105.17	110.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	601	NAG	O7-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	601	NAG	4	0
7	C	608	NAG	1	0
9	C	619	MAN	1	0
9	C	624	MAN	2	0
9	C	625	MAN	2	0
7	C	635	NAG	2	0
7	C	636	NAG	2	0
9	C	639	MAN	2	0
9	C	641	MAN	2	0
7	C	653	NAG	1	0
7	D	702	NAG	2	0
8	D	703	BMA	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	230/239 (96%)	0.96	41 (17%) <b>2</b> <b>7</b>	341, 372, 429, 440	0
2	B	204/211 (96%)	0.28	17 (8%) <b>14</b> <b>18</b>	341, 387, 420, 424	0
3	C	447/480 (93%)	0.11	9 (2%) <b>68</b> <b>63</b>	302, 327, 347, 360	0
4	D	132/142 (92%)	0.05	1 (0%) <b>87</b> <b>83</b>	307, 317, 336, 349	0
5	E	224/238 (94%)	0.71	34 (15%) <b>3</b> <b>8</b>	307, 349, 400, 413	0
6	F	212/215 (98%)	0.38	18 (8%) <b>13</b> <b>17</b>	307, 347, 390, 397	0
All	All	1449/1525 (95%)	0.39	120 (8%) <b>14</b> <b>18</b>	302, 342, 413, 440	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	199	SER	9.4
1	A	126	PRO	7.0
5	E	201	VAL	6.8
5	E	198	SER	6.7
5	E	159	CYS	6.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	NAG	E	301	14/15	0.72	0.55	4.39	316,316,316,316	0
7	NAG	C	603	14/15	0.76	0.36	2.70	329,329,329,329	0
7	NAG	C	616	14/15	0.72	0.47	1.34	337,337,337,337	0
9	MAN	C	619	11/12	0.93	0.23	0.56	340,340,340,340	0
7	NAG	C	615	14/15	0.57	0.33	0.22	349,349,349,349	0
9	MAN	E	306	11/12	0.81	0.30	0.06	339,339,339,339	0
9	MAN	E	305	11/12	0.73	0.33	-0.04	335,335,335,335	0
9	MAN	C	624	11/12	0.55	0.31	-0.08	342,342,342,342	0
7	NAG	C	659	14/15	0.88	0.24	-0.09	335,335,335,335	0
7	NAG	C	626	14/15	0.92	0.30	-0.13	342,342,342,342	0
7	NAG	C	642	14/15	0.78	0.34	-0.19	344,344,344,344	0
7	NAG	C	607	14/15	0.92	0.21	-0.35	334,334,334,334	0
7	NAG	D	701	14/15	0.83	0.25	-0.51	313,313,313,313	0
7	NAG	C	635	14/15	0.89	0.32	-0.78	327,327,327,327	0
9	MAN	C	625	11/12	0.82	0.15	-0.98	345,345,345,345	0
9	MAN	E	310	11/12	0.86	0.17	-1.24	330,330,330,330	0
7	NAG	C	627	14/15	0.93	0.13	-2.04	350,350,350,350	0
7	NAG	C	608	14/15	0.90	0.15	-2.23	341,341,341,341	0
8	BMA	C	661	11/12	0.77	0.33	-	365,365,365,365	0
9	MAN	C	634	11/12	0.86	0.29	-	365,365,365,365	0
7	NAG	C	651	14/15	0.54	0.56	-	389,389,389,389	0
8	BMA	C	609	11/12	0.71	0.16	-	348,348,348,348	0
7	NAG	C	636	14/15	0.94	0.28	-	333,333,333,333	0
8	BMA	C	620	11/12	0.73	0.28	-	337,337,337,337	0
9	MAN	E	307	11/12	0.89	0.50	-	326,326,326,326	0
9	MAN	C	618	11/12	0.91	0.25	-	336,336,336,336	0
9	MAN	C	645	11/12	0.84	0.27	-	407,407,407,407	0
9	MAN	E	308	11/12	0.95	0.32	-	325,325,325,325	0
7	NAG	E	302	14/15	0.91	0.42	-	318,318,318,318	0
7	NAG	C	602	14/15	0.68	0.77	-	342,342,342,342	0
7	NAG	C	654	14/15	0.69	0.27	-	376,376,376,376	0
9	MAN	D	704	11/12	0.93	0.28	-	343,343,343,343	0
9	MAN	C	633	11/12	0.87	0.14	-	359,359,359,359	0
9	MAN	C	613	11/12	0.80	0.35	-	361,361,361,361	0
9	MAN	C	612	11/12	0.65	0.23	-	361,361,361,361	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MAN	C	646	11/12	0.79	0.21	-	417,417,417,417	0
8	BMA	C	649	11/12	0.69	0.29	-	383,383,383,383	0
8	BMA	C	644	11/12	0.83	0.29	-	391,391,391,391	0
7	NAG	C	653	14/15	0.59	0.35	-	370,370,370,370	0
8	BMA	C	658	11/12	0.49	0.25	-	387,387,387,387	0
7	NAG	C	656	14/15	0.85	0.29	-	350,350,350,350	0
9	MAN	E	311	11/12	0.84	0.56	-	348,348,348,348	0
8	BMA	D	703	11/12	0.88	0.18	-	328,328,328,328	0
7	NAG	C	604	14/15	0.72	0.46	-	342,342,342,342	0
9	MAN	C	639	11/12	0.69	0.35	-	346,346,346,346	0
8	BMA	C	655	11/12	0.71	0.27	-	386,386,386,386	0
9	MAN	C	640	11/12	0.85	0.25	-	348,348,348,348	0
7	NAG	D	705	14/15	0.79	0.34	-	327,327,327,327	0
9	MAN	C	638	11/12	0.84	0.65	-	350,350,350,350	0
7	NAG	C	605	14/15	0.93	0.21	-	354,354,354,354	0
7	NAG	C	650	14/15	0.78	0.64	-	378,378,378,378	0
8	BMA	C	628	11/12	0.89	0.11	-	354,354,354,354	0
7	NAG	C	601	14/15	0.88	0.28	-	334,334,334,334	0
7	NAG	C	660	14/15	0.93	0.17	-	351,351,351,351	0
9	MAN	C	623	11/12	0.94	0.35	-	346,346,346,346	0
8	BMA	C	652	11/12	0.65	0.35	-	401,401,401,401	0
9	MAN	C	610	11/12	0.87	0.26	-	352,352,352,352	0
7	NAG	C	648	14/15	0.87	0.22	-	374,374,374,374	0
9	MAN	E	304	11/12	0.91	0.42	-	332,332,332,332	0
9	MAN	E	309	11/12	0.94	0.58	-	334,334,334,334	0
8	BMA	E	303	11/12	0.77	0.44	-	326,326,326,326	0
9	MAN	C	641	11/12	0.63	0.37	-	349,349,349,349	0
9	MAN	C	611	11/12	0.83	0.35	-	364,364,364,364	0
9	MAN	C	621	11/12	0.93	0.28	-	338,338,338,338	0
7	NAG	C	606	14/15	0.83	0.28	-	364,364,364,364	0
7	NAG	C	647	14/15	0.90	0.26	-	354,354,354,354	0
7	NAG	C	643	14/15	0.82	0.30	-	366,366,366,366	0
9	MAN	C	622	11/12	0.75	0.25	-	341,341,341,341	0
9	MAN	C	632	11/12	0.94	0.13	-	359,359,359,359	0
7	NAG	C	657	14/15	0.88	0.26	-	371,371,371,371	0
7	NAG	D	702	14/15	0.92	0.14	-	319,319,319,319	0
8	BMA	C	637	11/12	0.84	0.35	-	341,341,341,341	0
9	MAN	C	614	11/12	0.89	0.18	-	367,367,367,367	0
9	MAN	C	630	11/12	0.75	0.29	-	357,357,357,357	0
9	MAN	C	631	11/12	0.83	0.36	-	367,367,367,367	0
9	MAN	C	629	11/12	0.75	0.17	-	357,357,357,357	0
7	NAG	C	617	14/15	0.87	0.29	-	341,341,341,341	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.